

Relativistic mixed-sector intermediate hamiltonian coupled cluster method: theory and applications

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Newly developed mixed-sector relativistic multireference Coupled Cluster (CC) scheme based on Intermediate Hamiltonian formulation is presented. This formulation widely extends possibilities of the traditional Fock-space and Hilbert-space CC approaches and could be regarded as a bridge between the two approaches. High-precision calculations of some heavy and super-heavy atomic systems are presented. The new method yields converged results for states not accessible by traditional Relativistic Fock-space coupled cluster approach. Moreover, states calculated by both methods exhibit much better accuracy in the mixed-sector intermediate Hamiltonian (MSIH) formulation.